Introduction to Machine Learning

Feature Selection

Andres Mendez-Vazquez

February 19, 2019

Outline

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What is this?

Main Question

“Given a number of features, how can one select the most important of them so as to reduce their number and at the same time retain as much as possible of their class discriminatory information? “

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2. if information-rich features are selected, the design of the classifier can be greatly simplified.

- Large between-class distance.
- Small within-class variance.

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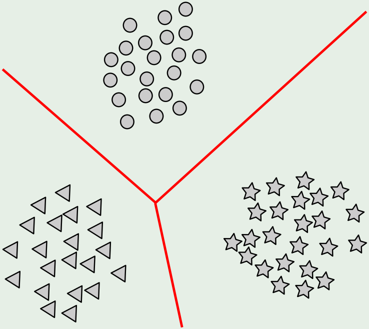
Basically, we want nice separated and dense clusters!!!



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It is necessary to do the following

1. Outlier removal.
2. Data normalization.
3. Deal with missing data.

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You can do the following

1. If you have a small number $\Rightarrow$ discard them!!!
2. Adopt cost functions that are not sensitive to outliers:
   1. For example, possibilistic clustering.
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Algorithm

Input: An $N \times d$ data set $Data$

Output: Candidate Outliers

1. Calculate the sample mean μ and sample covariance matrix Σ.
2. Let M be $N \times 1$ vector consisting of square of the Mahalonobis distance to μ.
3. Find points O in M whose values are greater than

$$\chi^2_d(0.05)$$

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How?

Get the Sample Mean per feature k

$$\boldsymbol{m}_i = \frac{1}{N}\sum_{k=1}^{N} \boldsymbol{x}_{ki}$$

Get the Sample Variance per feature k

$$v_i = \frac{1}{N-1}\sum_{k=1}^{N} \left(\boldsymbol{x}_{ki} - \boldsymbol{m}_i\right)\left(\boldsymbol{x}_{ki} - \boldsymbol{m}_i\right)^T$$

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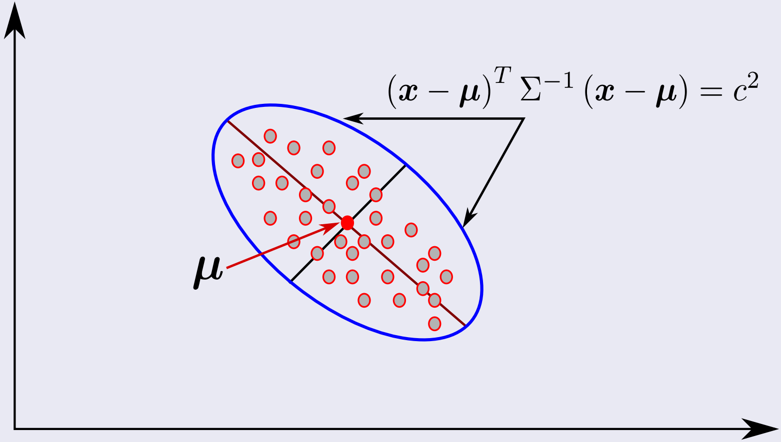
Mahalonobis Distance

We have

$$M(\boldsymbol{x}) = \sqrt{(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})}$$

Thus

Setting $M(\boldsymbol{x})$ to a constant c defines a multidimensional ellipsoid with centroid at $\boldsymbol{\mu}$



Algorithm

The Partial Code

```
def OutlierRemoval(self, Data):
        SampleMean  = Data.mean(1)
        SampleCov   = Data - SampleMean
        SampleCov   = np.cov(SampleCov.T)
        Mahalonobis = (Data - SampleMean)*
                                    np.inv(SampleCov)*
                                    ((Data - SampleMean).T)

        # Something else here
        # Here you can use chi2.isf(\alpha,dim)
```

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Data Normalization

In the real world

In many practical situations a designer is confronted with features whose values lie within different dynamic ranges.

For Example

We can have two features with the following ranges

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\begin{aligned}
x_i &\in [0, 100, 000] \\
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Features with large values may have a larger influence in the cost function than features with small values.

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Be Naive

For each feature $i = 1, ..., d$ obtain the $\max_i$ and the $\min_i$ such that

$$\hat{x}_{ik} = \frac{x_{ik} - \min_i}{\max_i - \min_i} \tag{1}$$

Problem

This simple normalization will send everything to a unitary sphere thus loosing data resolution!!!

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Example III

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All new features have zero mean and unit variance.

Further

Other linear techniques limit the feature values in the range of $[0, 1]$ or $[-1, 1]$ by proper scaling.

However

We can non-linear mapping. For example the softmax scaling.

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Softmax Scaling

It consists of two steps

First one

$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{3}$$

Second one

$$\hat{x}_{ik} = \frac{1}{1 + \exp\left\{-y_{ik}\right\}} \tag{4}$$

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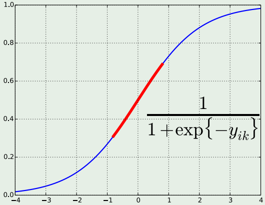
Explanation

Notice the red area is almost flat!!!



Thus, we have that

- The red region represents values of y inside of the region defined by the mean and variance (small values of y).
- Then, if we have those values x behaves as a linear function.

And values too away from the mean

They are squashed by the exponential part of the function.

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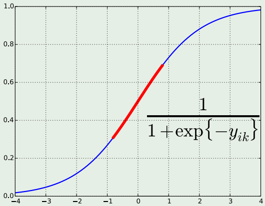

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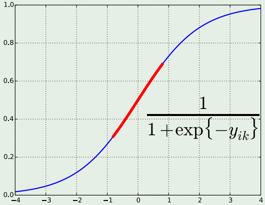

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This can happen

In practice, certain features may be missing from some feature vectors.

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Some traditional techniques to solve this problem

Use zeros and risked it!!!

The idea is not to add anything to the features

The sample mean/unconditional mean

Does not matter what distribution you have use the sample mean

$$\overline{x}_i = \frac{1}{N}\sum_{k=1}^{N} x_{ik} \tag{5}$$

Find the distribution of your data

Use the mean from that distribution. For example, if you have a beta distribution

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The MOST traditional

Drop it

- Remove that data
  - Still you need to have a lot of data to have this luxury

Something more advanced

Split data samples in two set of variables

$$\boldsymbol{x}_{complete} = \begin{pmatrix} \boldsymbol{x}_{observed} \\ \boldsymbol{x}_{missed} \end{pmatrix} \tag{7}$$

Generate the following probability distribution

$$P\left(\boldsymbol{x}_{missed} | \boldsymbol{x}_{observed}, \Theta\right) = \frac{P\left(\boldsymbol{x}_{missed}, \boldsymbol{x}_{observed} | \Theta\right)}{P\left(\boldsymbol{x}_{observed} | \Theta\right)} \tag{8}$$

where

$$p\left(\boldsymbol{x}_{observed} | \Theta\right) = \int_{\mathcal{X}} p\left(\boldsymbol{x}_{complete} | \Theta\right) d\boldsymbol{x}_{missed} \tag{9}$$

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Something more advanced - A two step process

Clearly the Θ needs to be calculated

For this, we use the Expectation Maximization Algorithm (Look at it for that)

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Then, using Monte Carlo methods

We draw samples from (Something as simple as slice sampler)

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What?

The intuition, the larger the number of samples vs the number of features, the smaller the error P_e

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Graphically

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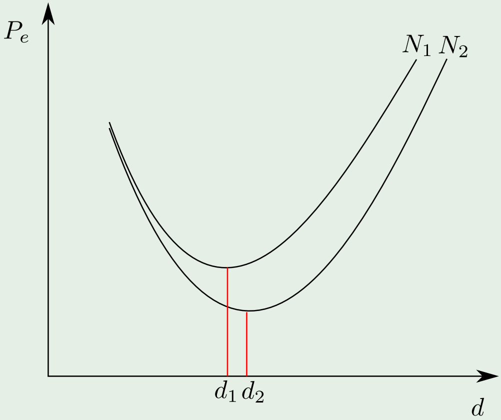

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Given N

d must be large enough to learn what makes classes different and what makes patterns in the same class similar

In addition

d must be small enough not to learn what makes patterns of the same class different

In practice

In practice, $d < N/3$ has been reported to be a sensible choice for a number of cases

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In practice, $d < N/3$ has been reported to be a sensible choice for a number of cases

Back to Feature Selection

Given N

d must be large enough to learn what makes classes different and what makes patterns in the same class similar

In addition

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Once d has been decided, choose the d most informative features:

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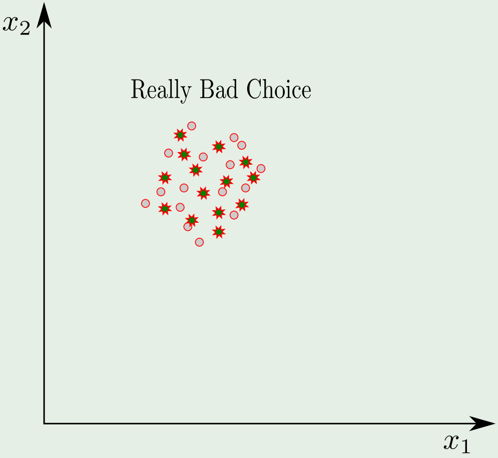
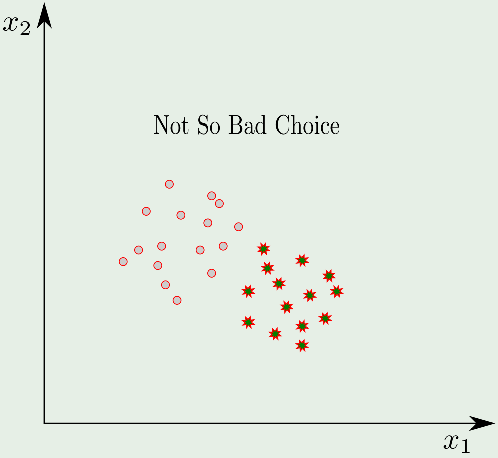
Example

Thus, we want to avoid choices



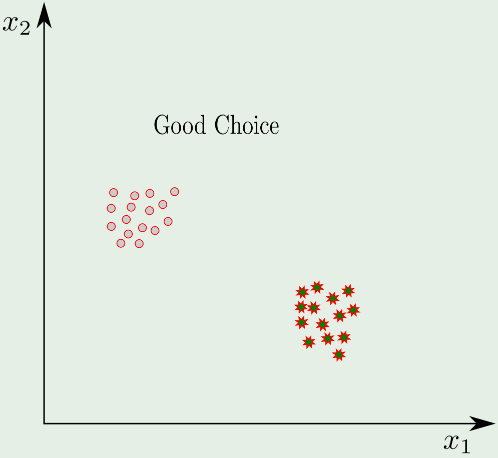
Example

Better Choice



Example

What We Want to Have



Outline

Considering Feature Sets

Something Notable

The emphasis so far was on individually considered features.

But

That is, two features may be rich in information, but if they are highly correlated we need not consider both of them.

Then

Combine features to search for the "best" combination after features have been discarded.

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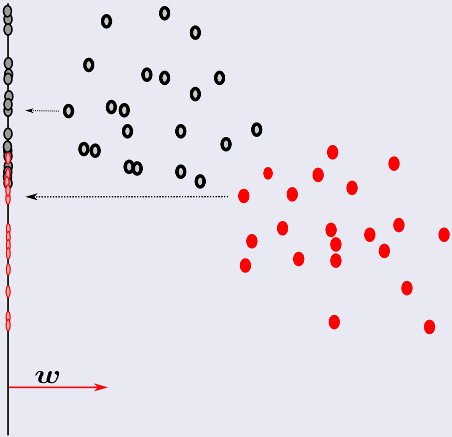

A Better Line

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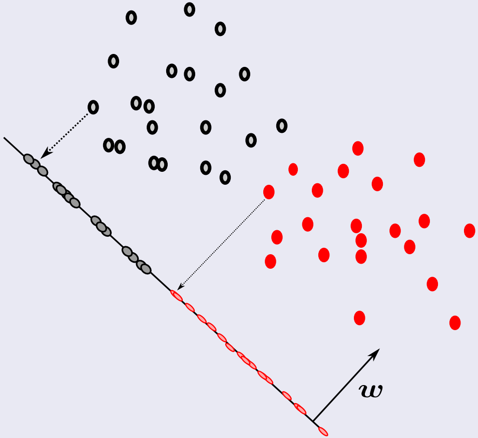

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where C is the number of classes.

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The global mean.

Mixture scatter matrix

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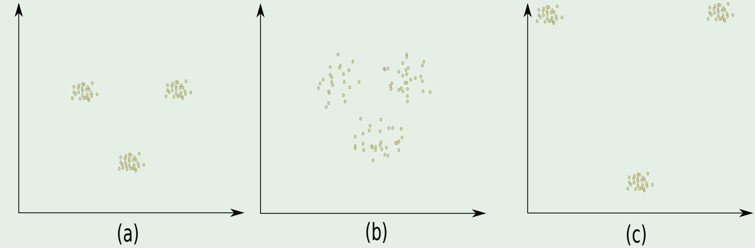
(a) small within-class variance and small between-class distances, (b) large within-class variance and small between-class distances, and (c) small within-class variance and large between-class distances.



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We want to avoid

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Given x_1, x_2, x_3, x_4 and we wish to select two of them

Step 1

Adopt a class separability criterion, C, and compute its value for the feature vector $[x_1, x_2, x_3, x_4]^T$.

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